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13. ABSTRACT (Maximum 200 words)

This research involves theoretical studies of the chemical and fluid-mechanical phenomena which make turbulent combustion in high-speed flows different from such combustion in low-speed flows. Finite-rate chemistry plays a significant role in high-speed flows because of the small ratios of flow times to chemical times. The studies address ignition and extinction phenomena in nonpremixed turbulent combustion of hydrogen-air systems by both numerical and asymptotic methods. Attention also is paid to effects of compressibility in high-speed turbulent combustion, with consideration given to interdispersal configurations of shocklets and flamelets. Efforts are made to provide a firmer foundation for the modeling of high-speed turbulent reacting flows, to aid in the development of a formulation which gives results that can be compared with experiments on turbulent combustion.

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INTRODUCTION

Uncertainties about turbulent combustion in hydrogen-air systems have an impact on our abilities to achieve successful designs of supersonic combustion devices for the National Aerospace Plane, for example. Prior to initiation of the present research, it was not known whether the combustion was more likely to occur in reaction-sheet or distributed-reaction regimes, and common practice was to assume the latter and employ laminar chemical kinetics in routines based on computational fluid mechanics. As will be seen below, estimates suggest that this is a poor procedure since the reaction-sheet regime is more prevalent than the distributed-reaction regime. The present research was initiated because it was felt desirable to try to determine the regimes more firmly and to develop improved methods for accounting for the chemical kinetics of the combustion.

RESEARCH OBJECTIVES

The objective of this research is to improve understanding of the chemical kinetics and fluid dynamics of turbulent combustion in high-speed flows. At present emphasis is being placed on understanding the ignition processes in nonpremixed counterflow systems of hydrogen and air. In addition, to understand the effects of heat release on the high-speed compressible turbulence on direct numerical simulation study is also being initiated. The results may help to improve abilities to design propulsion systems that employ high-speed turbulent combustion.

ACCOMPLISHMENTS

The previous annual report described research on ignition in hydrogen-air mixtures, on nonpremixed flames in stagnating turbulence and on structures of counterflow diffusion flames with small stoichiometric mixture fractions. The complete reference citation for publication of the work on the last of these topics was not available last year and therefore is included here as the first reference. The present discussion focuses on the new research performed during the past year. This research emphasizes ignition phenomena as well as extinction, introduces methods of bifurcation theory and offers some experimental measurements to test theoretical predictions.

This research emphasizes the flamelet regime of turbulent diffusion flames. It is important to use the most up-to-date information to assess whether applications are most likely to fall in flamelet (flame-sheet) or distributed-reaction regimes. Such assessments have recently been completed for hypersonic propulsion employing hydrogen-air diffusion flames, and the results support continued emphasis on the flamelet regime. Attention was thus focused on flamelets in the hydrogen-air system, and four separate studies presently underway are reported here, all of them involving counterflowing configurations in one way or another.

Numerical Investigation of Ignition in Hydrogen-Air Mixtures

The critical parameters and the structure of the ignition kernel in hydrogen-air nonpremixed counterflowing configurations were calculated for a range of pressures from 0.5 to 40 atmospheres, for a range of initial temperatures and for a range of equivalence ratio. The conservation equations for the counterflow system with an updated chemical mechanism were numerically integrated using the arc-tracing continuation technique. The results of such complete calculations are not only useful for assessing the adequateness of various approximate models required in theoretical modeling and in large-scale simulation of these flames, but also provide guidance for combustor designers concerning the ranges of operations in which the ignition is controlling.

Representative results for the peak temperature as a function of the strain rate show that the extinction strain rate for hydrogen flames, unlike that for methane flames, is seen to increase rapidly with increasing pressure. These results are consistent with the dependences of the crossover temperatures on the pressures for the two fuels. The crossover temperature for hydrogen flames is the temperature at which the rate of the chain branching reaction $H + O_2 \rightarrow OH + O$ becomes equal to that of the chain termination step $H + O_2 + M \rightarrow HO_2 + M$, while for methane flame the rate of the branching step is to be compared with the rate of the radical-removing step $CH_4 + H \rightarrow CH_3 + H_2$, which is bimolecular rather than three-body.

The critical strain rate for ignition is seen to be very sensitive to the oxidizer temperature. Above a transition value of the oxidizer temperature, no abrupt ignition or extinction phenomena are observed. This transition temperature, which is slightly larger than the crossover temperature for reasons discussed below, is calculated along with the corresponding transition strain rate as a function of pressure. As the oxidizer temperature is reduced the critical ignition strain rate decreases rapidly and soon reaches values where the convective effects of the flowfield have a minimal influence on the ignition processes. In addition, the middle branch of the S-curve is seen to approach the frozen branch increasingly tangentially with decreasing oxidizer temperature. It is extremely difficult to determine the ignition strain rate accurately by the continuation method for these cases; the solutions are extremely sensitive to the initial conditions and may converge to the middle branch. It is uncertain whether any currently available computational approach can circumvent this difficulty and attention is being given to this question.

Another application of the results from full integrations relates to the assessment of reduced mechanisms for the treatment of hydrogen oxidation in practical devices. In the calculation of multidimensional problems, it is computationally desirable to reduce the number of species that must be taken into account. A four-step mechanism was obtained by imposing steady-state approximations for HO_2 and H_2O_2. Three different three-step mechanism results from the four-step scheme by introducing a steady-state approximation for O or OH, or by employing steady states for both O and OH simultaneously and relaxing the HO_2 steady-state assumption. Finally a two-step mechanism is obtained by putting all species except H in steady state. Results were obtained for the peak temperature as a function of the strain rate, according to the prediction of the full and these reduced chemical schemes for a diluted hydrogen-air diffusion flame at atmospheric pressure; results are similar without dilution. It is found that the two-step chemistry gives higher maximum temperature consistent with

the higher H concentration predicted by the two-step chemistry in the reaction zone, yet the extinction and ignition strain rates differ only by approximately 10% and 15%, respectively for the undiluted flames and up to 25% and 40%, respectively for extreme dilutions (15% molar concentration of H_2 in the fuel stream.) It is interesting to observe that the discrepancy between the predictions of the two-step and full-mechanisms arises largely from the O steady-state assumption. On the other hand, calculations imposing H steady-state with the O steady-state relaxed gave results too poor to plot on the figure, thus suggesting that though the ignition may occur far on the air side of the mixing layer, the attack of H-atoms on O_2 (the chain-branching step) still plays a dominant role in initiating and propagating the ignition process. These results are being published.

Asymptotic Analysis of the Ignition Processes in Hydrogen-Air System

In a theoretical study, the slope of the ignition branch for steady, counterflow, hydrogen-oxygen diffusion flames, with dilution permitted in both streams, was investigated for two-step reduced chemistry by methods of bifurcation theory. Attention was restricted to fuel-stream temperatures less than or equal to the oxidizer-stream temperature T_∞ and to T_∞ larger than or of the order of the crossover temperature at which the rates of the $H + O_2$ chain-branching and chain-terminating steps are equal. Two types of solutions were identified, a frozen solution that always exists in this kinetic approximation because all rates are proportional to the concentration of the intermediate H atom, and an ignited solution that bifurcates from the frozen solution if a Damköhler number constructed from the strain rate and the rate of the branching step $H + O_2 \rightarrow OH + O$ is increased to a critical value at which the strain rate becomes small enough for autoignition to occur in this flow field. Along the ignited branch, the original two-step chemistry soon fails near the hot oxidizer stream, necessitating consideration of $O + H_2 \rightarrow OH + O$ as the dominant chain-branching step, the effect of which was included in the analysis by introducing a finite position of H_2 depletion, with frozen flow beyond, to the oxidizer boundary. The critical Damköhler number for ignition, and the slope of the curve of the maximum radical concentration as a function of Damköhler at the ignition point, were calculated parametrically as functions of the hydrogen Lewis number, and different limiting behaviors were clarified for Lewis numbers of zero and unity. It was shown that when effects of chemical heat release are neglected, so that the ignition involves only a branched-chain explosion, a good approximation at sufficiently high T_∞, the ignition is always gradual in the sense that the limiting ignited-branch slope is positive (supercritical bifurcation) and there is no S curve. At high T_∞ the radical-production step alone affords a good one-step approximation for ignition, but its heat release is too small to remove the gradual-ignition behavior, even as T_∞ drops below crossover. Near crossover it becomes necessary to include the radical-consumption step as well, while which is much more exothermic, and even before crossover the augmentation of the branched-ch ain explosion by its associated heat release readily produces abrupt ignition, a negati ve limiting ignition-branch slope (subcritical bifurcation) which leads to an S curve. For T_∞ somewhat below crossover, the branched-chain contribution to igniti on ceases entirely, and a thermal-explosion character must develop. The results are a first step towards analytical description of nonpremixed H_2-O_2 autoignition. This work is being published.

Experimental Investigation of Hydrogen-Air Diffusion Flames

Most of the research on hydrogen-air diffusion flames has been of a theoretical or numerical nature. Very few experiments have been performed to test the detailed numerical diffusion-flame models. To remedy this deficiency, an experimental investigation was initiated to ascertain how well the chemical-kinetic mechanism which has been used in the present work for the hydrogen-oxygen-nitrogen systems can predict measured diffusion-flame extinction conditions. The results from this study show that the measurements and computations of extinction strain rates for an axisymmetric counterflow configuration agree very well for diluted flames. Experimental data begin to depart from theory at the highest hydrogen mole fractions shown because of the onset of experimental difficulties that prevent good tests from being made at higher hydrogen concentrations. The results of these studies have been accepted for publication.

Nonpremixed Flames in Stagnating Turbulence

Our analysis of nonpremixed flames in stagnating turbulence is continuing. The principal focus of this study is the comparison of theory with the experimental results or methane-air flames reported by the Whitelaw Group at Imperial College. Since these flames occupy approximately 40% of the gap between the two jets carrying the turbulent fuel and oxidizer streams, the thin flame analysis used in all previous treatments of flames in stagnating turbulence is inapplicable and a new approach based on solving the conservation equations from one exit plane to the other has been developed. Our present fluid mechanical treatment is based on the $k - \epsilon$ theory while a presumed pdf-flame sheet description is used to deal with the chemistry. The numerical analysis of the resulting system of ordinary differential equations is extremely difficult but solutions have now been obtained and compared with experimental data. In making the comparison with the available data, we confront the problem of dealing with predictions based on Favre-averaging and experimental data presumably involving conventional averaging. Thus in the present case only fluid mechanical quantities in the two constant density regions outside of the flame and the state variables within the flame are subject to comparison. Somewhat surprising is the finding of qualitative agreement with the former data but excellent agreement with the latter. We intend to conclude this study and then apply the theory to hydrogen-air flames perhaps with a Reynolds stress theory for the description of the fluid mechanical behavior.

PUBLICATIONS

1. J. S. Kim and F. A. Williams. Structures of flow and mixture fraction fields for counterflow diffusion flames with small stoichiometric mixture fractions. *SIAM Journal on Applied Mathematics*, 53(6):1551–1566, December 1993.

2. G. Balakrishnan and F. A. Williams. Turbulent combustion regimes for hypersonic propulsion employing hydrogen-air diffusion flames. *Journal of Propulsion and Power*, to appear, 1994.

3. G. Balakrishnan, M. D. Smooke, and F. A. Williams. A numerical investigation of the ignition and extinction limits in laminar nonpremixed counterflowing hydrogen-air streams. *Combustion and Flame*, submitted, 1994.

4. A. Sánchez, A. Liñán, and F. A. Williams. A bifurcation analysis of high-temperature ignition of H_2 - O_2 diffusion flames. *Twenty-Fifth Symposium (International) on Combustion*, to appear, 1994.

5. G. Balakrishnan, D. Trees, and F. A. Williams. An experimental investigation of strain-induced extinction of diluted hydrogen-air counterflow diffusion flames. *Combustion and Flame*, to appear, 1994.

PERSONNEL

			Percentage Time
Prof. P.A. Libby	Prin. Investigator	100%, May 1993 only =	8% annually
Prof. F.A. Williams	Prin. Investigator	Summer only (3 months) =	20%
G. Balakrishnan	Postgrad. Researcher		100%
N. Ilincic	PhD Student	50% Mar. & Apr. 1993 =	8% annually

INTERACTIONS

Related talks given by the PIs at meetings and at visits during the reporting period are:

"Supercritical Combustion of Multicomponent Droplets," Phillips Lab, Edwards AFB, March 5, 1993

"How Asymptotic Concepts Can Help in Estimating Pollutant Production in Turbulent Diffusion Flames," University of Illinois, Department of Mechanical & Industrial Engineering, April 12, 1993

"Theories of Turbulent Combustion in High Speed Flows" and "Fundamental Acoustic Instability in Liquid Propellant Rockets," AFOSR mtg, Atlantic City, New Jersey June 14-18, 1993

"The Role of Hydrogen-Air Diffusion Flamelets in Hypersonic Propulsion" University of Virginia, September 9-10, 1993

"Reduced Chemistry for Hydrogen-Air Supersonic Combustion," UC Los Angeles, November 19, 1993

INVENTIONS

None.